

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 1.27e-01

Global applicability domain: Inside

Local applicability domain index: 6.66e-01

Confidence level: 7.20e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>1-Propanol</div> <div>Measured: 0.25</div> <div>Predicted: 1.27e-01</div>	<div>Image not found</div> <div>Propanol, 3-fluoro-</div> <div>Measured: -0.280</div> <div>Predicted: -0.00652</div>	<div>Image not found</div> <div>Isopropanol</div> <div>Measured: 0.05</div> <div>Predicted: 2.58e-01</div>
<div>Image not found</div> <div>1-Butanol</div> <div>Measured: 0.88</div> <div>Predicted: 8.38e-01</div>	<div>Image not found</div> <div>1,4-Butanediol</div> <div>Measured: -0.830</div> <div>Predicted: -0.621</div>	